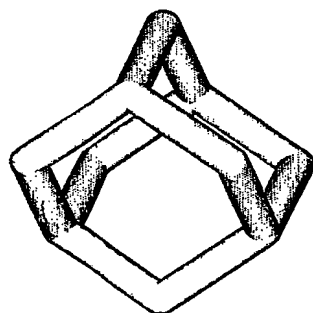
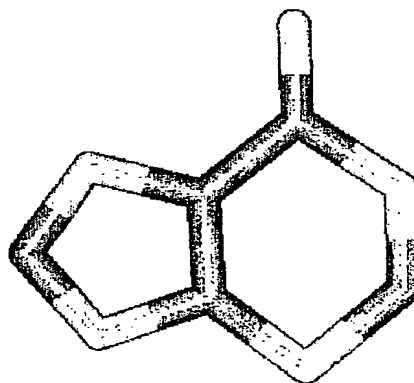


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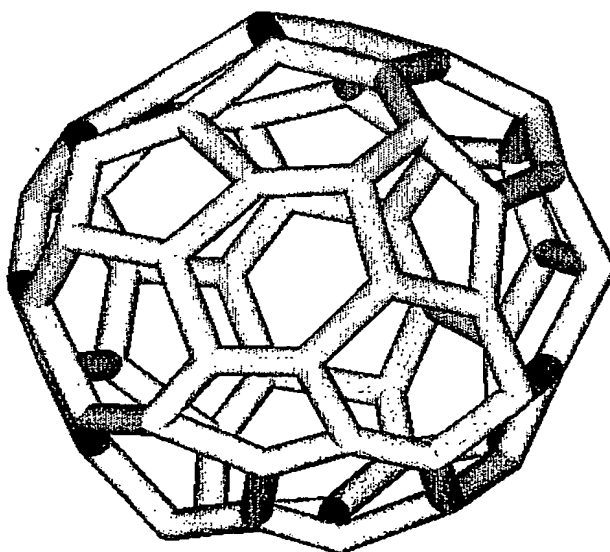
adamantane (RMSD = 0.04Å)

FIG.1 A



adenine (RMSD = 0.12Å)

FIG.1 B



fullerene (RMSD = 0.24Å)

FIG.1 C

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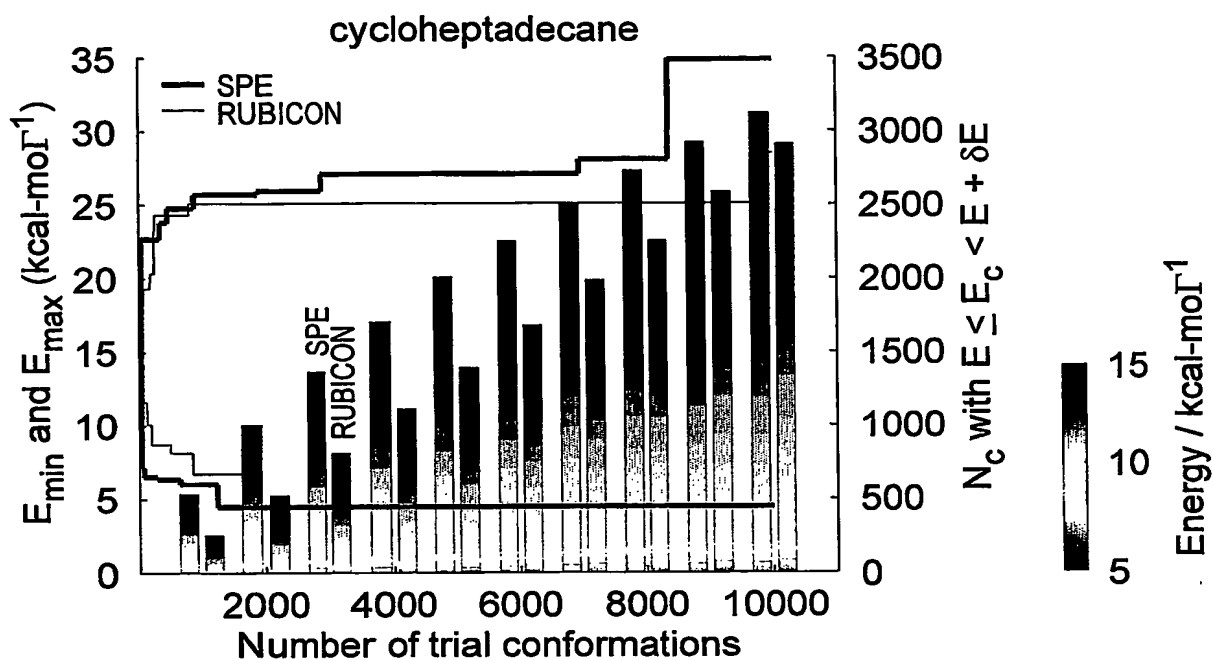


FIG.2A

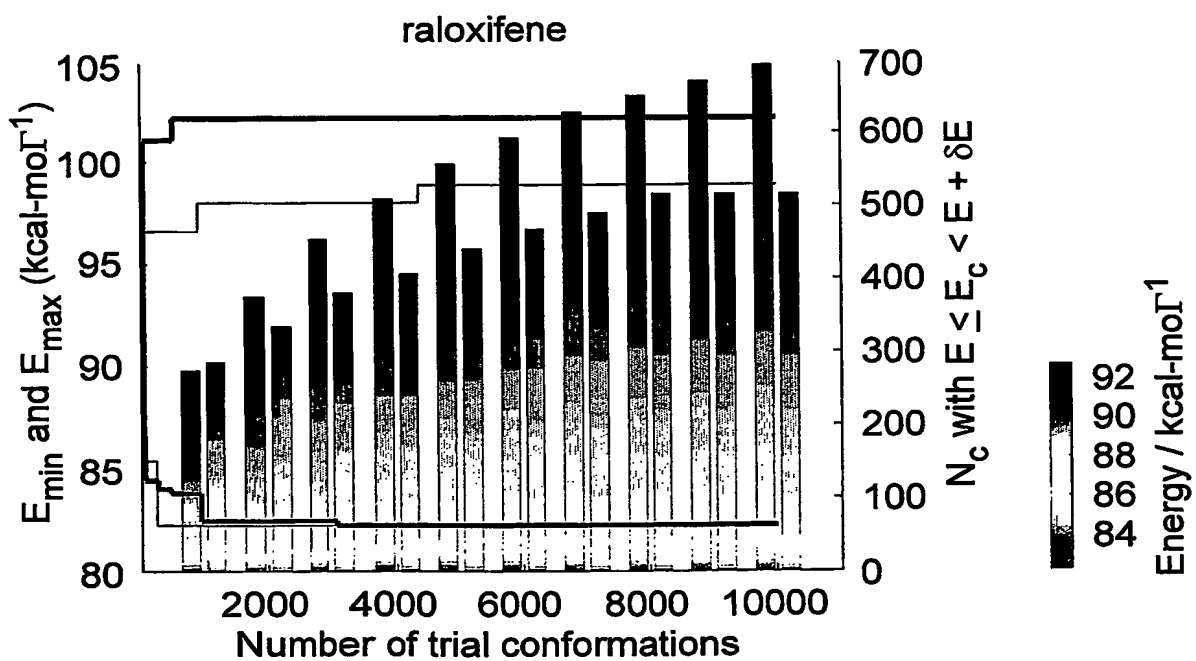


FIG.2B

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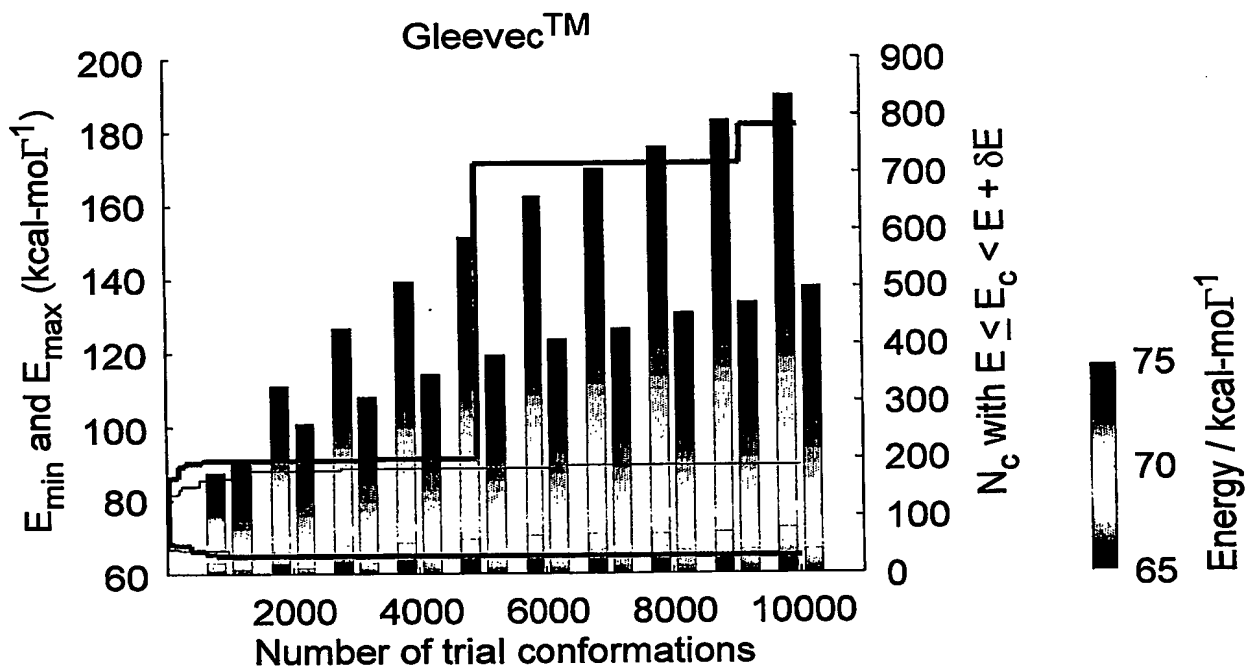


FIG.2C

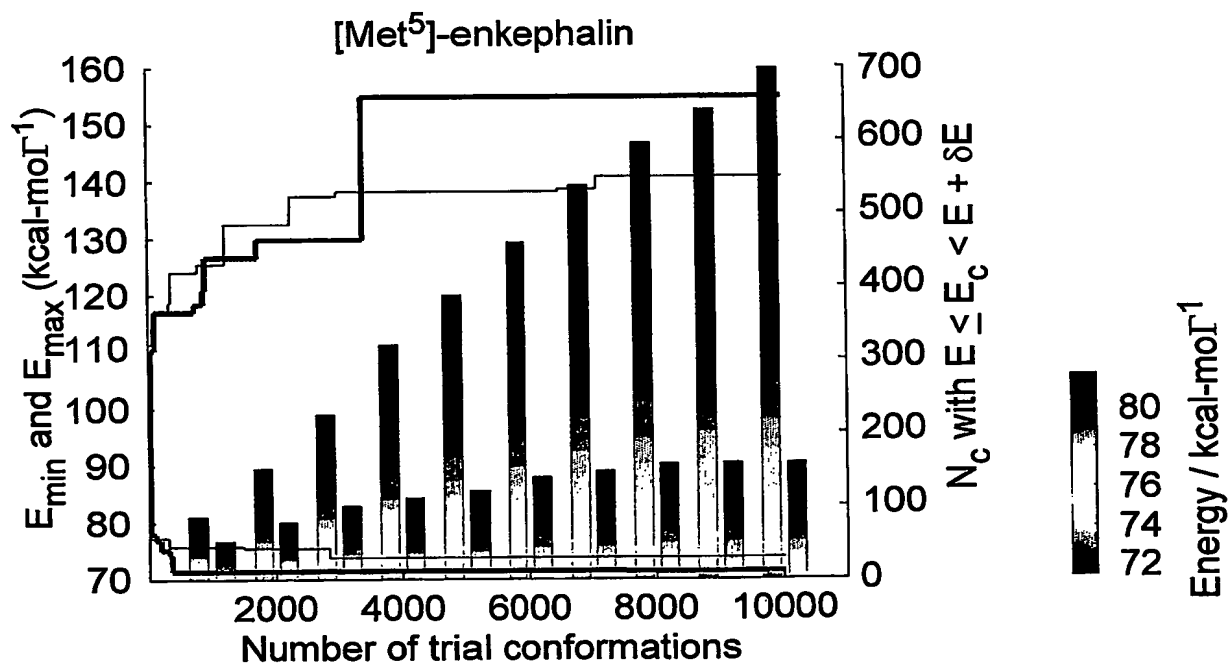


FIG.2D

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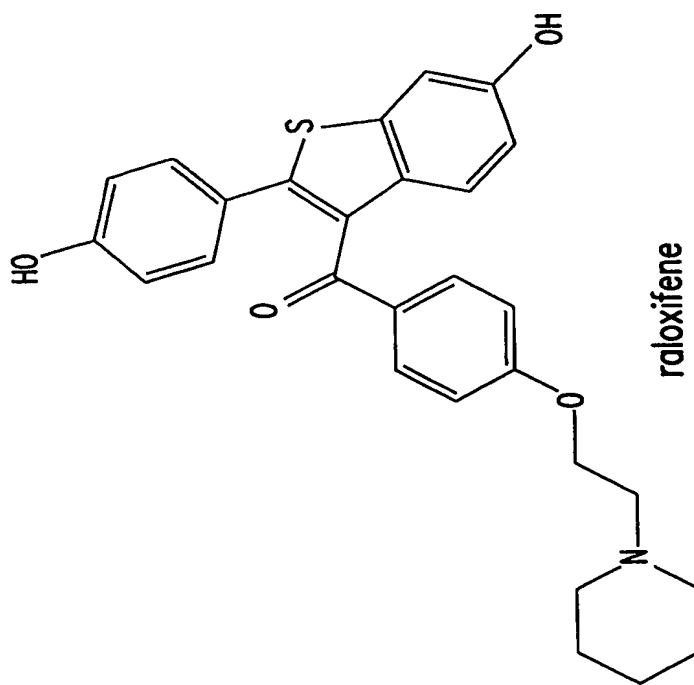


FIG. 3A

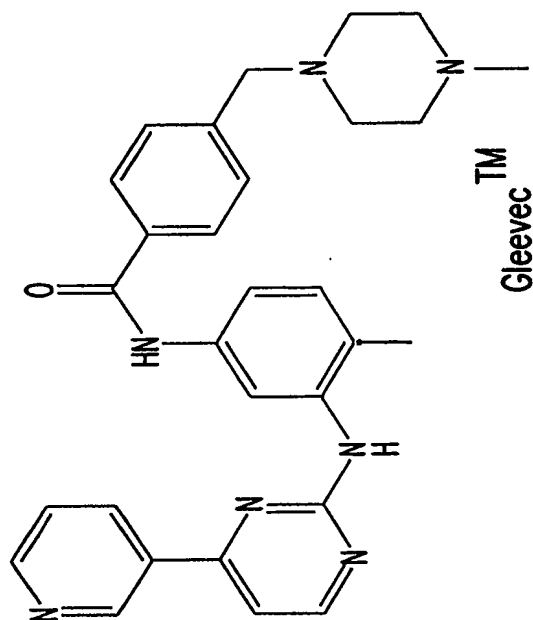
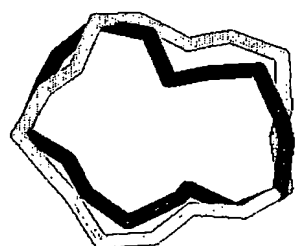


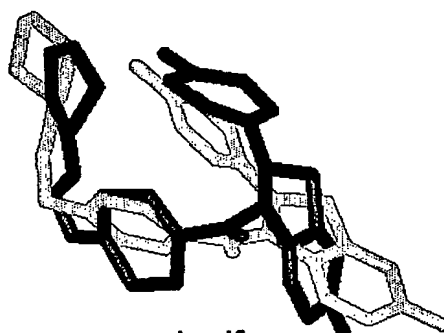
FIG. 3B

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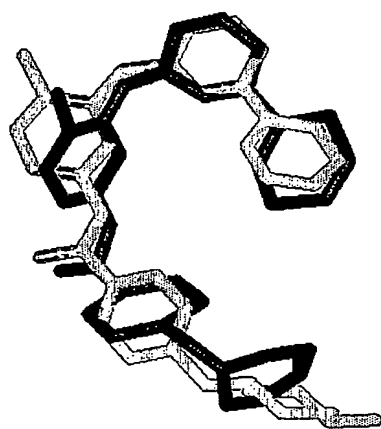
cycloheptadecane
(RMSD=0.90Å)

FIG.3C



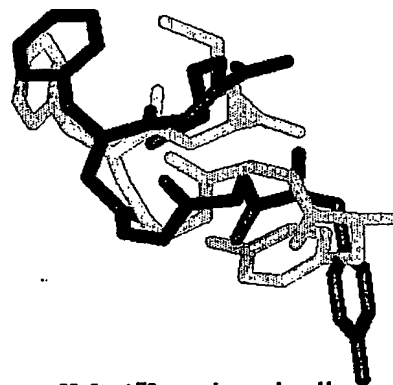
raloxifene
(RMSD=1.51Å)

FIG.3D



Gleevec™
(RMSD=1.69Å)

FIG.3E



[Met⁵]-enkephalin
(RMSD=2.43Å)

FIG.3F

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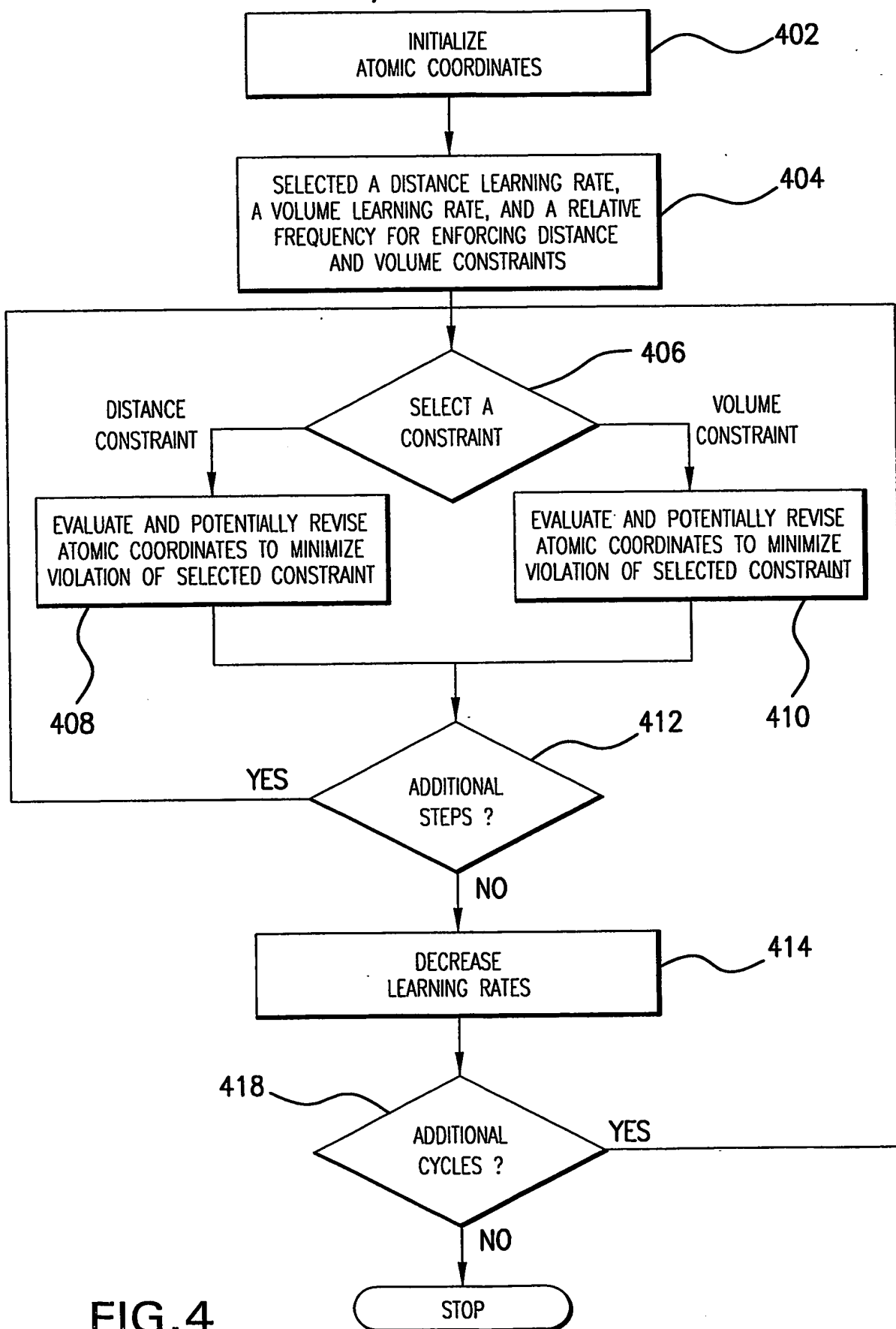


FIG. 4

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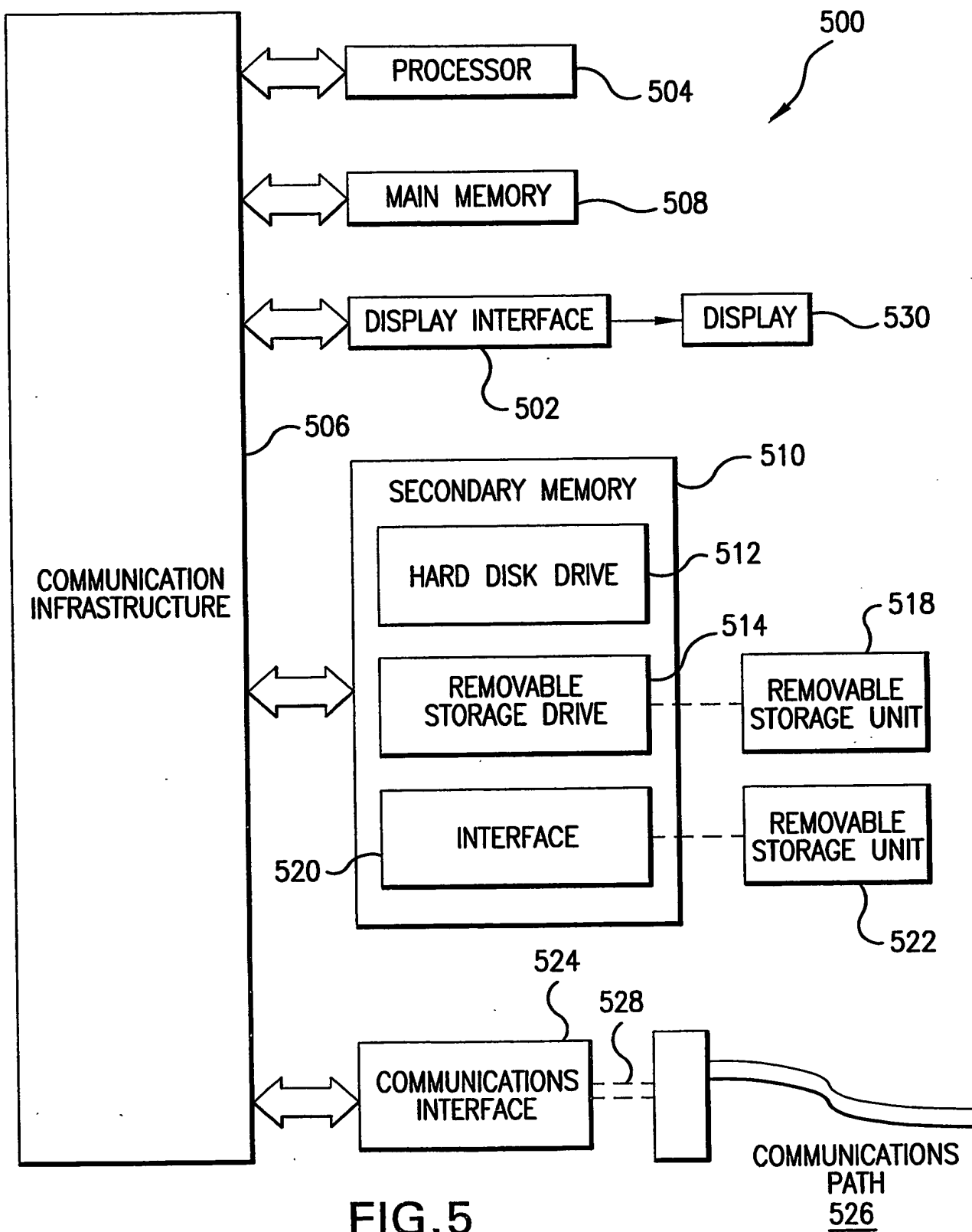


FIG. 5

MOLECULE	t_{SPE} (sec)	t_{RUBICON} (sec)	n_d^{SPE}	n_d^{RUBICON}	$E_{\text{min}}^{\text{SPE}}$ (kcal·mol ⁻¹)	$E_{\text{min}}^{\text{RUBICON}}$ (kcal·mol ⁻¹)
cycloheptadecane	0.049	0.615	5908	4453	4.5105	4.5105
raloxifene	0.242	1.215	1915	689	82.2486	82.2486
Gleevec TM	0.261	1.677	3482	1228	64.8114	64.8482
[Met ⁵]- enkephalin	0.306	1.819	9995	8019	71.3763	73.8235

TABLE 1

FIG.6